Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Antiferromagnetism in GaS monolayer doped with TM-TM pair (TM = V, Cr, Mn, and Fe)

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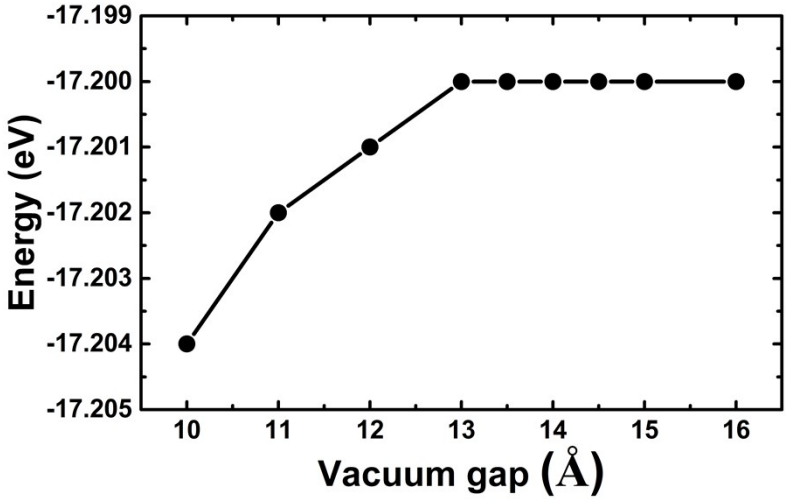

Figure S1: Vacuum-dependent variation of energy of GaS monolayer.

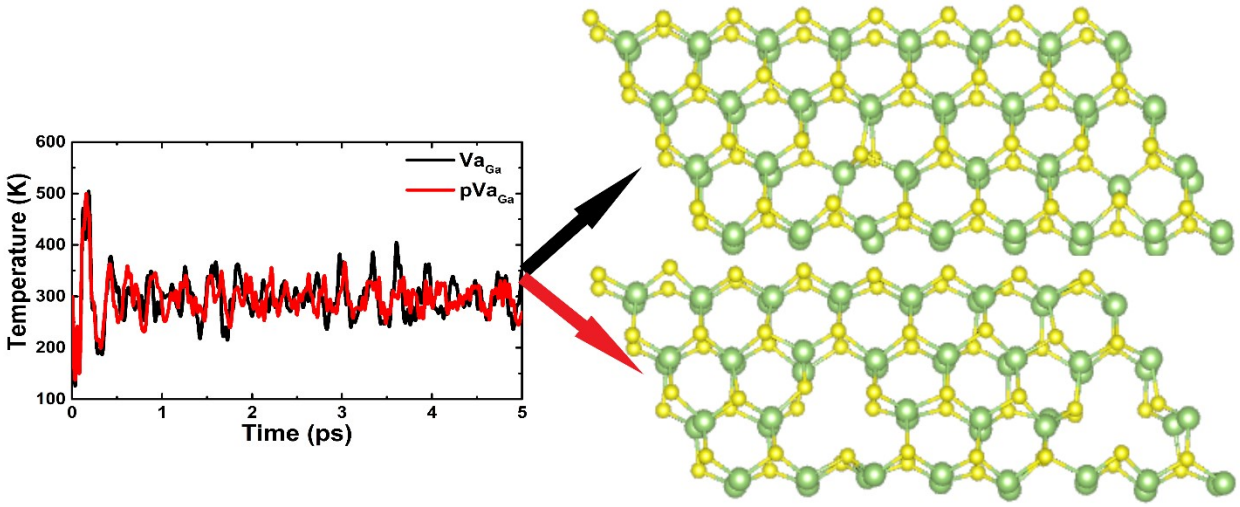

Figure 2: AIMD simulations at 300 K (Variation of temperature + Atomic structure after 5 ps of simulations) of Va_{Ga} and pVa_{Ga} systems.

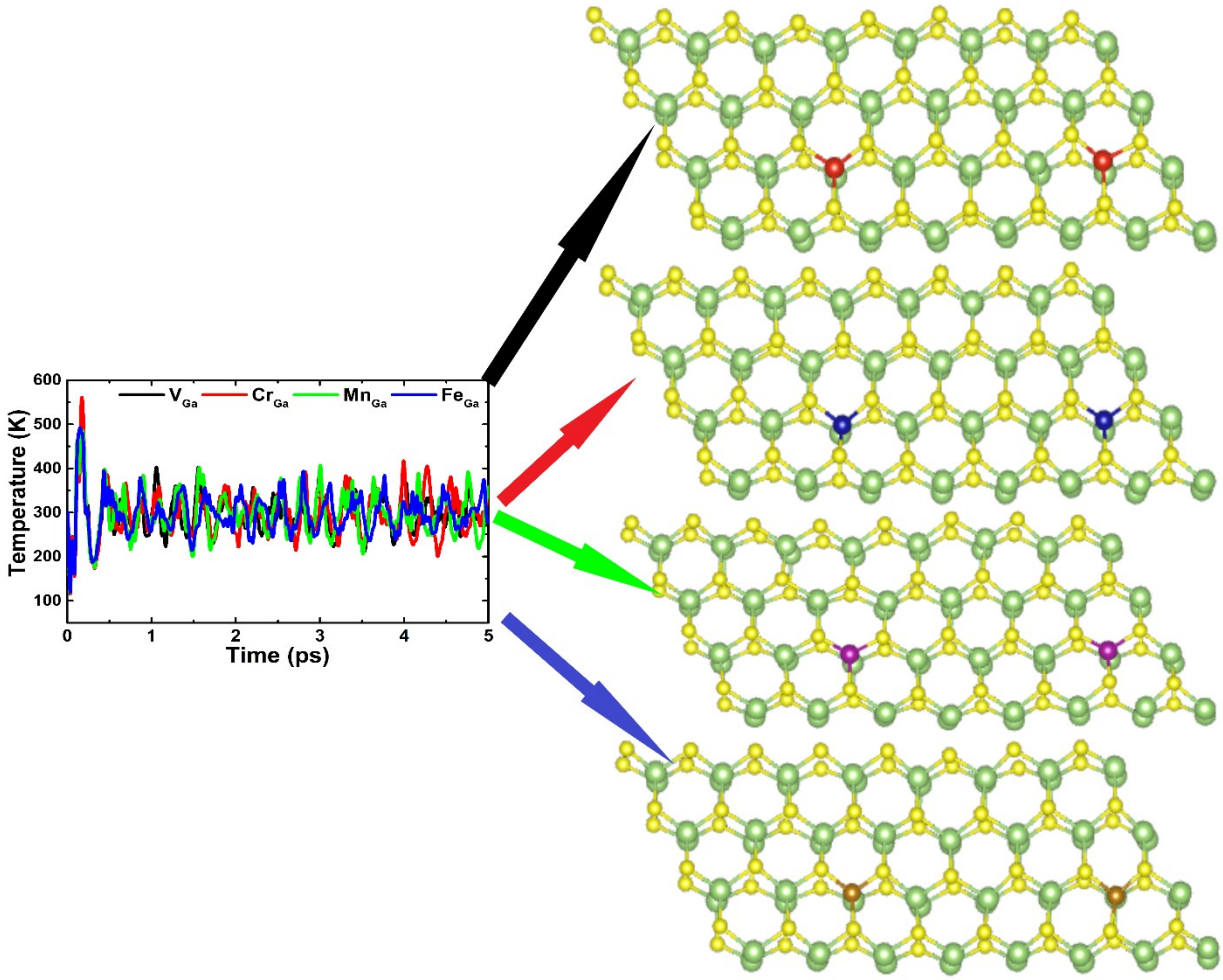

Figure 3: AIMD simulations at 300 K (Variation of temperature + Atomic structure after 5 ps of simulations) of V_{Ga}, Cr_{Ga}, Mn_{Ga}, and Fe_{Ga} systems.

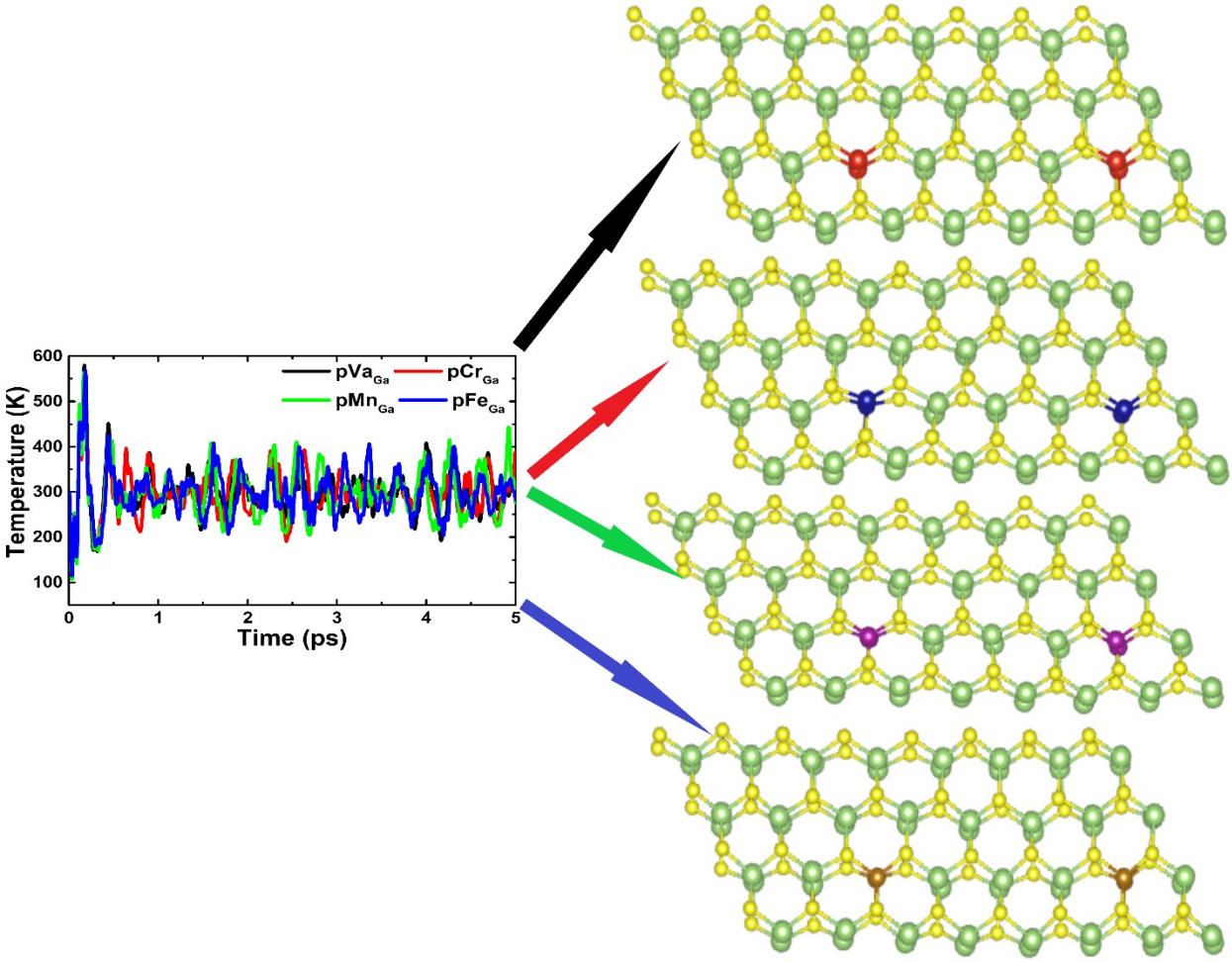

Figure 4: AIMD simulations at 300 K (Variation of temperature + Atomic structure after 5 ps of simulations) of pV_{Ga}, pCr_{Ga}, pMn_{Ga}, and pFe_{Ga} systems.

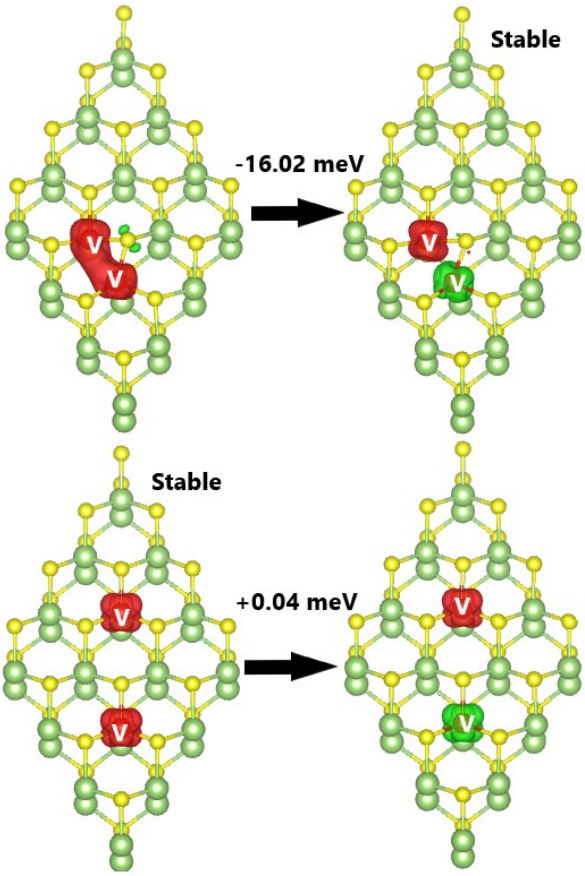

Figure S5: Spin density (Iso-surface value: 0.01 e/Å^3; Red surface: Spin-up; Green surface: Spin-down) in GaS monolayer in-plane-doped with V atoms with different interatomic distances.

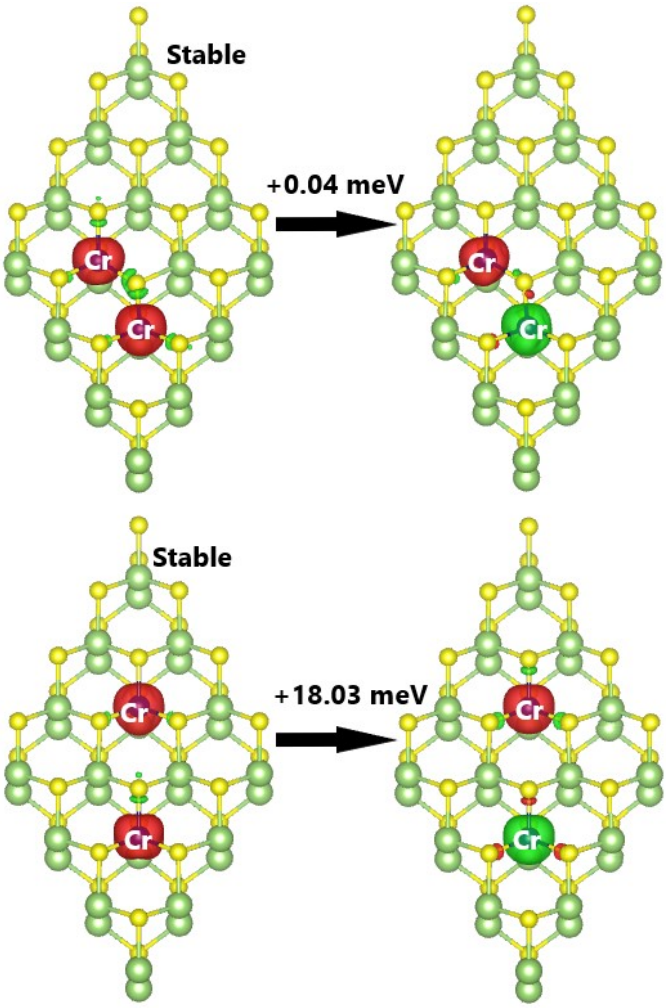

Figure S6: Spin density (Iso-surface value: 0.01 e/Å^3; Red surface: Spin-up; Green surface: Spin-down) in GaS monolayer in-plane-doped with Cr atoms with different interatomic distances.

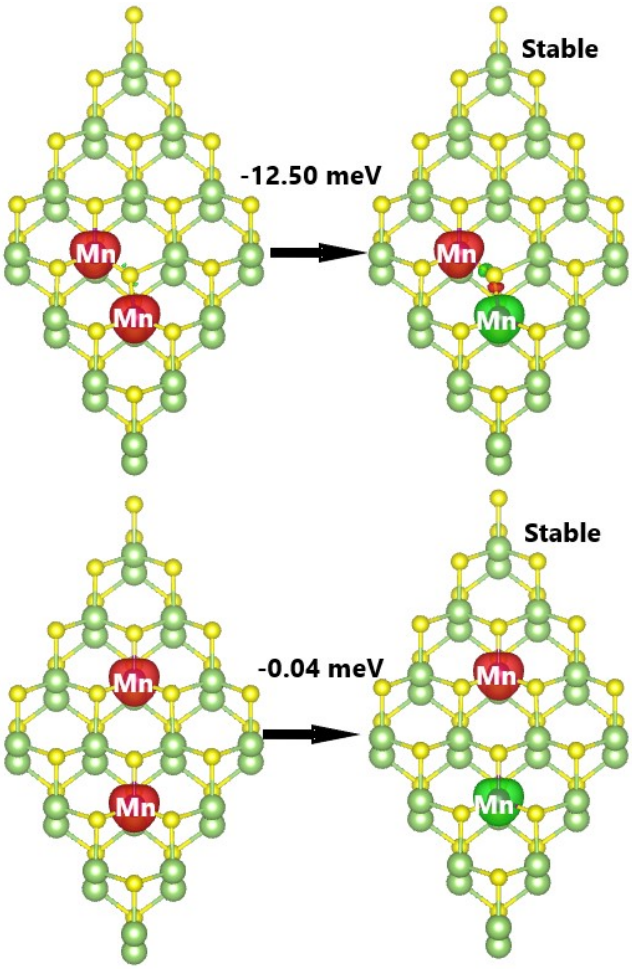

Figure S7: Spin density (Iso-surface value: 0.01 e/Å^3; Red surface: Spin-up; Green surface: Spin-down) in GaS monolayer in-plane-doped with Mn atoms with different interatomic distances.

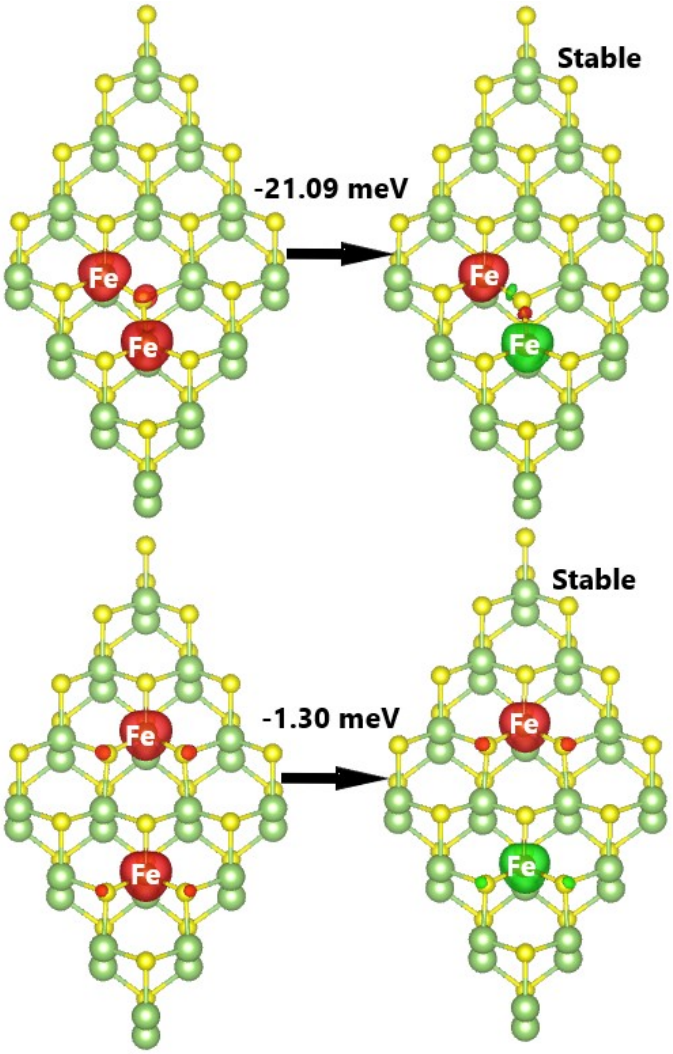

Figure S8: Spin density (Iso-surface value: 0.01 e/Å^3; Red surface: Spin-up; Green surface: Spin-down) in GaS monolayer in-plane-doped with Fe atoms with different interatomic distances.